



ELSEVIER

Chemical Physics 256 (2000) 363–366

Chemical
Physics

www.elsevier.nl/locate/chemphys

Author index

- Adamovich, I.V., see Plönjes, E. 256 (2000) 315
Alikhani, M.E., see Asselin, P. 256 (2000) 195
Allouche, A.R., see Korek, M. 256 (2000) 1
- Asselin, P., P. Soulard, M.E. Alikhani and J.P. Perchard, Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and supersonic jet-FTIR experiments 256 (2000) 195
Aubert-Frécon, M., see Korek, M. 256 (2000) 1
- Babinec, P., see Roszak, S. 256 (2000) 177
Baer, T., see Kim, D. 256 (2000) 251
Baraille, I., see Dupin, H. 256 (2000) 7
Baumgärtel, H., see Hoxha, A. 256 (2000) 239
Billard, I., see Bockstahl, F. 256 (2000) 307
Blaise, P., and O. Henri-Rousseau, Spectral density of medium strength H-bonds. Direct damping and intrinsic anharmonicity of the slow mode. Beyond adiabatic approximation 256 (2000) 85
Bockstahl, F., E. Pachoud, G. Duplâtre and I. Billard, Size of sodium dodecyl sulphate micelles in aqueous NaCl solutions as studied by positron annihilation lifetime spectroscopy 256 (2000) 307
Bruno, D., see Longo, S. 256 (2000) 265
- Cassidei, L., see Petrella, G. 256 (2000) 259
Chaalan, A., see Korek, M. 256 (2000) 1
Chae, W.-S., see Kang, S.-G. 256 (2000) 295
Chen, X.J., see Zhang, C.F. 256 (2000) 275
Chernukho, A.P., see Plönjes, E. 256 (2000) 315
Cho, B.R., see Kim, S. 256 (2000) 289
Choi, J.-H., Spectral properties and ligand field analysis of *cis*-dinitrito(1,4,8,11-tetraazacyclotetradecane)chromium(III) nitrate 256 (2000) 29
Christophorov, L.N., A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik, Structure-function self-organization in nonequilibrium macromolecular systems 256 (2000) 45
Ciriaco, F., see Petrella, G. 256 (2000) 259
Cong, S.-L., K.-L. Han, G.-Z. He and N.-Q. Lou, Determination of population, orientation and alignment of symmetric top molecule using laser-induced fluorescence 256 (2000) 225

Congeduti, A., M. Nardone and P. Postorino, Polarized Raman spectra of a single crystal of iodine	256 (2000) 117
Costela, A., see Holzer, W.	256 (2000) 125
Dagher, M., see Korek, M.	256 (2000) 1
Dargelos, A., see Dupin, H.	256 (2000) 7
Dehareng, D., see Hoxha, A.	256 (2000) 239
Doetschman, D.C., D.C. Gilbert and D.W. Dwyer, Li cation–aromatic organic radical complex in a zeolite studied by electron spin echo envelope modulation spectroscopy	256 (2000) 37
Duarte, F.J., see Holzer, W.	256 (2000) 125
Dupin, H., I. Baraille, C. Larrieu and A. Dargelos, Theoretical study of the infrared and ultraviolet spectrum of the radical F_2CN	256 (2000) 7
Duplâtre, G., see Bockstahl, F.	256 (2000) 307
Dwyer, D.W., see Doetschman, D.C.	256 (2000) 37
Elstner, M., K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and S. Suhai, DFT studies on helix formation in N -acetyl-(L-alanyl) $_n$ -N'-methylamide for $n = 1$ –20	256 (2000) 15
Fakherddin, K., see Korek, M.	256 (2000) 1
Frauenheim, Th., see Elstner, M.	256 (2000) 15
García-Moreno, I., see Holzer, W.	256 (2000) 125
Gauduel, Y., and H. Gelabert, Primary steps of an electron–proton reaction in aqueous electrolyte solutions	256 (2000) 333
Gelabert, H., see Gauduel, Y.	256 (2000) 333
Gilbert, D.C., see Doetschman, D.C.	256 (2000) 37
Goez, M., and V. Zubarev, Light intensity dependence of a two-photon catalytic cycle: photoionization via absorption–electron transfer–absorption	256 (2000) 107
Gratz, H., see Holzer, W.	256 (2000) 125
Han, K.-L., see Cong, S.-L.	256 (2000) 225
Harris, K.D.M., see Turner, G.W.	256 (2000) 159
He, G.-Z., see Cong, S.-L.	256 (2000) 225
Henri-Rousseau, O., see Blaise, P.	256 (2000) 85
Holzer, W., H. Gratz, T. Schmitt, A. Penzkofer, A. Costela, I. García-Moreno, R. Sastre and F.J. Duarte, Photo-physical characterization of rhodamine 6G in a 2-hydroxyethyl-methacrylate methyl-methacrylate copolymer	256 (2000) 125
Holzwarth, A.R., see Christoparov, L.N.	256 (2000) 45
Hottmann, K., see Hoxha, A.	256 (2000) 239
Hoxha, A., R. Locht, B. Leyh, D. Dehareng, K. Hottmann and H. Baumgärtel, Photoelectron spectroscopy of vinylbromide and intramolecular dynamics of the ionic \tilde{B} state	256 (2000) 239
Hwang, D.-Y., and A.M. Mebel, Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide	256 (2000) 169
Hwang, J., see Kim, S.	256 (2000) 289
Itkin, A.L., Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers	256 (2000) 61

- Jalkanen, K.J., see Elstner, M. 256 (2000) 15
 Johnston, R.L., see Turner, G.W. 256 (2000) 159
 Jung, J.-S., see Kang, S.-G. 256 (2000) 295
 Jurczok, M., P. Plaza, W. Rettig and M.M. Martin, Ultrafast electron transfer in acceptor substituted bianthryl derivatives 256 (2000) 137
- Kang, S.-G., W.-S. Chae, Y.-R. Kim, J.-S. Jung and S.-H. Lee, Electronic energy dynamics of photoexcited ternary Zintl phase LiSbTe₂ and the distance estimation between trap sites 256 (2000) 295
 Kang, T.I., see Kim, S. 256 (2000) 289
 Kharkyanen, V.N., see Christophorov, L.N. 256 (2000) 45
 Kim, D., and T. Baer, Gas-phase measurement of ΔH^0 between axial and equatorial conformations of 3-methylcyclopentanone 256 (2000) 251
 Kim, S., H. Moon, J. Hwang, J. Sohn, J. Seo, S.Y. Park, T. I. Kang and B. R. Cho, First hyperpolarizabilities of dipolar photoconductive chromophores: an approach toward monolithic molecular materials for photorefractivity 256 (2000) 289
 Kim, Y.-R., see Kang, S.-G. 256 (2000) 295
 Knapp-Mohammady, M., see Elstner, M. 256 (2000) 15
 Kobeissi, M., see Korek, M. 256 (2000) 1
 Korek, M., A.R. Allouche, M. Kobeissi, A. Chaalan, M. Dagher, K. Fakherdin and M. Aubert-Frécon, Theoretical study of the electronic structure of the LiRb and NaRb molecules 256 (2000) 1
- Larrieu, C., see Dupin, H. 256 (2000) 7
 Lee, S.-H., see Kang, S.-G. 256 (2000) 295
 Leszczynski, J., see Roszak, S. 256 (2000) 177
 Leyh, B., see Hoxha, A. 256 (2000) 239
 Locht, R., see Hoxha, A. 256 (2000) 239
 Longo, S., D. Bruno and P. Minelli, Direct simulation of non-linear interparticle collisional relaxation of ensembles of two-level systems 256 (2000) 265
 Lou, N.-Q., see Cong, S.-L. 256 (2000) 225
- Martin, M.M., see Jurczok, M. 256 (2000) 137
 Mebel, A.M., see Hwang, D.-Y. 256 (2000) 169
 Minelli, P., see Longo, S. 256 (2000) 265
 Moon, H., see Kim, S. 256 (2000) 289
- Naguleswaran, S., M.F. Reid and G.E. Stedman, Prediction of pure electric-dipole two-photon absorption circular dichroism in lanthanide compounds 256 (2000) 207
 Nardone, M., see Congeduti, A. 256 (2000) 117
- Pachoud, E., see Bockstahl, F. 256 (2000) 307
 Palm, P., see Plönjes, E. 256 (2000) 315
 Park, S.Y., see Kim, S. 256 (2000) 289
 Penzkofer, A., see Holzer, W. 256 (2000) 125
 Perchard, J.P., see Asselin, P. 256 (2000) 195
 Petrella, G., L. Cassidei and F. Ciriaco, Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces 256 (2000) 259

Plönjes, E., P. Palm, A.P. Chernukho, I.V. Adamovich and J. William Rich, Time-resolved Fourier transform infrared spectroscopy of optically pumped carbon monoxide	256 (2000) 315
Plaza, P., see Jurczok, M.	256 (2000) 137
Postorino, P., see Congeduti, A.	256 (2000) 117
Reid, M.F., see Naguleswaran, S.	256 (2000) 207
Rettig, W., see Jurczok, M.	256 (2000) 137
Roszak, S., P. Babinec and J. Leszczynski, New phenomena revealed by quantum chemical studies – the shellvation of GeH_3^+ by H_2 molecules	256 (2000) 177
Sastre, R., see Holzer, W.	256 (2000) 125
Schmitt, T., see Holzer, W.	256 (2000) 125
Seo, J., see Kim, S.	256 (2000) 289
Sohn, J., see Kim, S.	256 (2000) 289
Soulard, P., see Asselin, P.	256 (2000) 195
Stampor, W., Electromodulation of fluorescence in hole-transporting materials (TPD, TAPC) for organic light-emitting diodes	256 (2000) 351
Starikov, E.B., Hartree-Fock crystal orbital calculation on sodium-intercalated fullerenes $\text{C}_{60}\text{Na}_{10}$ and $\text{C}_{60}\text{Na}_{11}$	256 (2000) 149
Stedman, G.E., see Naguleswaran, S.	256 (2000) 207
Suhai, S., see Elstner, M.	256 (2000) 15
Turner, G.W., R.L. Johnston and K.D.M. Harris, Systematic computational study of the geometrical dependence of deuterium quadrupole interaction parameters in an $\text{O}^- \text{H} \cdots \text{O}=\text{C}$ hydrogen bonded system	256 (2000) 159
van Mourik, F., see Christophorov, L.N.	256 (2000) 45
William Rich, J., see Plönjes, E.	256 (2000) 315
Xu, K.Z., see Zhang, C.F.	256 (2000) 275
Yuan, Z.S., see Zhang, C.F.	256 (2000) 275
Zarić, S.D., Theoretical study of cation- π interactions of the metal complex cation, $[\text{Co}(\text{NH}_3)_6]^{3+}$, with ethylene and acetylene	256 (2000) 213
Zhang, C.F., X.J. Chen, Z.S. Yuan, Z.J. Zhang and K.Z. Xu, Density functional theory studies of methylated uracil: geometries and energies	256 (2000) 275
Zhang, L., and M. Zhou, Theoretical investigation on the potential energy surface for the reactions of B, Al and Ga with NO	256 (2000) 185
Zhang, Z.J., see Zhang, C.F.	256 (2000) 275
Zhou, M., see Zhang, L.	256 (2000) 185
Zubarev, V., see Goez, M.	256 (2000) 107



Subject index

Methods and constructs

Theoretical

Computational methods for electronic structure

- DFT studies on helix formation in *N*-acetyl-(L-alanyl)_n-N'-methylamide for $n = 1\text{--}20$,
M. Elstner, K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and S. Suhai
Hartree-Fock crystal orbital calculation on sodium-intercalated fullerenes C₆₀Na₁₀ and
C₆₀Na₁₁, E.B. Starikov
- Systematic computational study of the geometrical dependence of deuterium quadrupole interaction parameters in an O–²H···O=C hydrogen bonded system, G.W. Turner, R.L. Johnston and K.D.M. Harris
- New phenomena revealed by quantum chemical studies – the shellvation of GeH₃⁺ by H₂ molecules, S. Roszak, P. Babinec and J. Leszczynski
- Theoretical study of cation–π interactions of the metal complex cation, [Co(NH₃)₆]³⁺, with ethylene and acetylene, S.D. Zarić

-CI and valence bond approach

- Theoretical study of the electronic structure of the LiRb and NaRb molecules, M. Korek, A.R. Allouche, M. Kobeissi, A. Chaalan, M. Dagher, K. Fakherdin and M. Aubert-Frécon
- Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide, D.-Y. Hwang and A.M. Mebel

-perturbative and many body approaches

- Theoretical study of the infrared and ultraviolet spectrum of the radical F₂CN, H. Dupin, I. Baraille, C. Larrieu and A. Dargelos
- Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide, D.-Y. Hwang and A.M. Mebel
- New phenomena revealed by quantum chemical studies – the shellvation of GeH₃⁺ by H₂ molecules, S. Roszak, P. Babinec and J. Leszczynski

-density functional theory

- DFT studies on helix formation in *N*-acetyl-(L-alanyl)_n-N'-methylamide for $n = 1\text{--}20$,
M. Elstner, K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and S. Suhai

Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide, D.-Y. Hwang and A.M. Mebel	256 (2000) 169
Theoretical investigation on the potential energy surface for the reactions of B, Al and Ga with NO, L. Zhang and M. Zhou	256 (2000) 185
Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and supersonic jet-FTIR experiments, P. Asselin, P. Soulard, M.E. Alikhani and J.P. Perchard	256 (2000) 195
Density functional theory studies of methylated uracil: geometries and energies, C.F. Zhang, X.J. Chen, Z.S. Yuan, Z.J. Zhang and K.Z. Xu	256 (2000) 275
<i>Semiempirical methods</i>	
DFT studies on helix formation in <i>N</i> -acetyl-(L-alanyl) _n -N'-methylamide for <i>n</i> = 1-20, M. Elstner, K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and S. Suhai	256 (2000) 15
Spectral properties and ligand field analysis of <i>cis</i> -dinitrito(1,4,8,11-tetraazacyclotetradecane)chromium(III) nitrate, J.-H. Choi	256 (2000) 29
First hyperpolarizabilities of dipolar photoconductive chromophores: an approach toward monolithic molecular materials for photorefractivity, S. Kim, H. Moon, J. Hwang, J. Sohn, J. Seo, S.Y. Park, T. Im Kang and B. Rae Cho	256 (2000) 289
<i>Spin states and magnetic interactions</i>	
Li cation-aromatic organic radical complex in a zeolite studied by electron spin echo envelope modulation spectroscopy, D.C. Doetschman, D.C. Gilbert and D.W. Dwyer	256 (2000) 37
<i>Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolarizabilities)</i>	
Prediction of pure electric-dipole two-photon absorption circular dichroism in lanthanide compounds, S. Naguleswaran, M.F. Reid and G.E. Stedman	256 (2000) 207
First hyperpolarizabilities of dipolar photoconductive chromophores: an approach toward monolithic molecular materials for photorefractivity, S. Kim, H. Moon, J. Hwang, J. Sohn, J. Seo, S.Y. Park, T. Im Kang and B. Rae Cho	256 (2000) 289
<i>Radiative (incl. relativistic) effects on molecules and molecular processes</i>	
Prediction of pure electric-dipole two-photon absorption circular dichroism in lanthanide compounds, S. Naguleswaran, M.F. Reid and G.E. Stedman	256 (2000) 207
<i>Reactive molecular dynamics including dissipative processes</i>	
Structure-function self-organization in nonequilibrium macromolecular systems, L.N. Christophorov, A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik	256 (2000) 45
<i>Molecular dynamics of many particle systems and condensed phases</i>	
Theoretical study of cation-π interactions of the metal complex cation, [Co(NH ₃) ₆] ³⁺ , with ethylene and acetylene, S.D. Zarić	256 (2000) 213
Determination of population, orientation and alignment of symmetric top molecule using laser-induced fluorescence, S.-L. Cong, K.-L. Han, G.-Z. He and N.-Q. Lou	256 (2000) 225

Quasiparticle dynamics (incl. excitons, polarons)

Electronic energy dynamics of photoexcited ternary Zintl phase LiSbTe₂ and the distance estimation between trap sites, S.-G. Kang, W.-S. Chae, Y.-R. Kim, J.-S. Jung and S.-H. Lee

256 (2000) 295

Statistical computational methods (incl. Monte Carlo)

Direct simulation of non-linear interparticle collisional relaxation of ensembles of two-level systems, S. Longo, D. Bruno and P. Minelli

256 (2000) 265

Dynamics of structures, lattices and macromolecular conformations

Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin

256 (2000) 61

Fluctuations and random processes

Structure-function self-organization in nonequilibrium macromolecular systems, L.N. Christophorov, A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik

256 (2000) 45

Non-equilibrium thermodynamic and hydrodynamic theories

Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin

256 (2000) 61

Time and space correlation functions

Spectral density of medium strength H-bonds. Direct damping and intrinsic anharmonicity of the slow mode. Beyond adiabatic approximation, P. Blaise and O. Henri-Rousseau

256 (2000) 85

Experiment*Magnetic resonances*

Li cation-aromatic organic radical complex in a zeolite studied by electron spin echo envelope modulation spectroscopy, D.C. Doetschman, D.C. Gilbert and D.W. Dwyer

256 (2000) 37

Direct simulation of non-linear interparticle collisional relaxation of ensembles of two-level systems, S. Longo, D. Bruno and P. Minelli

256 (2000) 265

Molecular spectroscopy

Spectral density of medium strength H-bonds. Direct damping and intrinsic anharmonicity of the slow mode. Beyond adiabatic approximation, P. Blaise and O. Henri-Rousseau

256 (2000) 85

Light intensity dependence of a two-photon catalytic cycle: photoionization via absorption-electron transfer-absorption, M. Goez and V. Zubarev

256 (2000) 107

Size of sodium dodecyl sulphate micelles in aqueous NaCl solutions as studied by positron annihilation lifetime spectroscopy, F. Bockstahl, E. Pachoud, G. Duplâtre and I. Billard

256 (2000) 307

Time-resolved Fourier transform infrared spectroscopy of optically pumped carbon monoxide, E. Plönjes, P. Palm, A.P. Chernukho, I.V. Adamovich and J. William Rich

256 (2000) 315

-infrared

- Spectral density of medium strength H-bonds. Direct damping and intrinsic anharmonicity of the slow mode. Beyond adiabatic approximation, P. Blaise and O. Henri-Rousseau
256 (2000) 85
- Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and supersonic jet-FTIR experiments, P. Asselin, P. Soulard, M.E. Alikhani and J.P. Perchard
256 (2000) 195
- Time-resolved Fourier transform infrared spectroscopy of optically pumped carbon monoxide, E. Plönjes, P. Palm, A.P. Chernukho, I.V. Adamovich and J. William Rich
256 (2000) 315
- Primary steps of an electron–proton reaction in aqueous electrolyte solutions, Y. Gauduel and H. Gelabert
256 (2000) 333

-Raman

- Polarized Raman spectra of a single crystal of iodine, A. Congeduti, M. Nardone and P. Postorino
256 (2000) 117

-UV

- Electromodulation of fluorescence in hole-transporting materials (TPD, TAPC) for organic light-emitting diodes, W. Stämpfli
256 (2000) 351

-visible

- Spectral properties and ligand field analysis of *cis*-dinitrito(1,4,8,11-tetraazacyclotetradecane)chromium(III) nitrate, J.-H. Choi
256 (2000) 29
- Electromodulation of fluorescence in hole-transporting materials (TPD, TAPC) for organic light-emitting diodes, W. Stämpfli
256 (2000) 351

Photoelectron and Auger spectroscopy

- Photoelectron spectroscopy of vinylbromide and intramolecular dynamics of the ionic $\tilde{\text{B}}$ state, A. Hoxha, R. Locht, B. Leyh, D. Dehareng, K. Hottmann and H. Baumgärtel
256 (2000) 239

Multiphoton ionization

- Gas-phase measurement of ΔH^0 between axial and equatorial conformations of 3-methylcyclopentanone, D. Kim and T. Baer
256 (2000) 251

Laser induced fluorescence

- Photo-physical characterization of rhodamine 6G in a 2-hydroxyethyl-methacrylate methyl-methacrylate copolymer, W. Holzer, H. Gratz, T. Schmitt, A. Penzkofer, A. Costela, I. Garcia-Moreno, R. Sastre and F.J. Duarte
256 (2000) 125
- Electronic energy dynamics of photoexcited ternary Zintl phase LiSbTe₂ and the distance estimation between trap sites, S.-G. Kang, W.-S. Chae, Y.-R. Kim, J.-S. Jung and S.-H. Lee
256 (2000) 295

Ultrafast measurements

- Ultrafast electron transfer in acceptor substituted bianthryl derivatives, M. Jurczok, P. Plaza, W. Rettig and M.M. Martin
256 (2000) 137
- Primary steps of an electron–proton reaction in aqueous electrolyte solutions, Y. Gauduel and H. Gelabert
256 (2000) 333

Nonlinear optics and spectroscopy

- Photo-physical characterization of rhodamine 6G in a 2-hydroxyethyl-methacrylate methyl-methacrylate copolymer, W. Holzer, H. Gratz, T. Schmitt, A. Penzkofer, A. Costela, I. García-Moreno, R. Sastre and F.J. Duarte 256 (2000) 125

Optical pumping

- Time-resolved Fourier transform infrared spectroscopy of optically pumped carbon monoxide, E. Plönjes, P. Palm, A.P. Chernukho, I.V. Adamovich and J. William Rich 256 (2000) 315

Atomic and molecular beam techniques

- Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco 256 (2000) 259

Light scattering

- First hyperpolarizabilities of dipolar photoconductive chromophores: an approach toward monolithic molecular materials for photorefractivity, S. Kim, H. Moon, J. Hwang, J. Sohn, J. Seo, S.Y. Park, T. Im Kang and B. Rae Cho 256 (2000) 289

Objects**Bulk systems***Gases*

- Theoretical study of the infrared and ultraviolet spectrum of the radical F_2CN , H. Dupin, I. Baraille, C. Larrieu and A. Dargelos 256 (2000) 7

- Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin 256 (2000) 61

- Gas-phase measurement of ΔH^0 between axial and equatorial conformations of 3-methylcyclopentanone, D. Kim and T. Baer 256 (2000) 251

- Direct simulation of non-linear interparticle collisional relaxation of ensembles of two-level systems, S. Longo, D. Bruno and P. Minelli 256 (2000) 265

- Time-resolved Fourier transform infrared spectroscopy of optically pumped carbon monoxide, E. Plönjes, P. Palm, A.P. Chernukho, I.V. Adamovich and J. William Rich 256 (2000) 315

Supersonic beams

- Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and supersonic jet-FTIR experiments, P. Asselin, P. Soulard, M.E. Alikhani and J.P. Perchard 256 (2000) 195

Liquid mixtures and solutions

- Ultrafast electron transfer in acceptor substituted bianthryl derivatives, M. Jurczok, P. Plaza, W. Rettig and M.M. Martin 256 (2000) 137

Crystals

- Hartree-Fock crystal orbital calculation on sodium-intercalated fullerenes $C_{60}Na_{10}$ and $C_{60}Na_{11}$, E.B. Starikov 256 (2000) 149

Prediction of pure electric-dipole two-photon absorption circular dichroism in lanthanide compounds, S. Naguleswaran, M.F. Reid and G.E. Stedman	256 (2000) 207
Electronic energy dynamics of photoexcited ternary Zintl phase LiSbTe ₂ and the distance estimation between trap sites, S.-G. Kang, W.-S. Chae, Y.-R. Kim, J.-S. Jung and S.-H. Lee	256 (2000) 295
<i>-neat</i>	
Polarized Raman spectra of a single crystal of iodine, A. Congeduti, M. Nardone and P. Postorino	256 (2000) 117
<i>-mixed</i>	
Hartree-Fock crystal orbital calculation on sodium-intercalated fullerenes C ₆₀ Na ₁₀ and C ₆₀ Na ₁₁ , E.B. Starikov	256 (2000) 149
<i>-micelles</i>	
Size of sodium dodecyl sulphate micelles in aqueous NaCl solutions as studied by positron annihilation lifetime spectroscopy, F. Bockstahl, E. Pachoud, G. Duplâtre and I. Billard	256 (2000) 307
<i>Polymers</i>	
Photo-physical characterization of rhodamine 6G in a 2-hydroxyethyl-methacrylate methyl-methacrylate copolymer, W. Holzer, H. Gratz, T. Schmitt, A. Penzkofer, A. Costela, I. Garcia-Moreno, R. Sastre and F.J. Duarte	256 (2000) 125
<i>Metals and alloys</i>	
Spectral properties and ligand field analysis of <i>cis</i> -dinitrito(1,4,8,11-tetraazacyclotetradecane)chromium(III) nitrate, J.-H. Choi	256 (2000) 29
<i>Thin films</i>	
Electromodulation of fluorescence in hole-transporting materials (TPD, TAPC) for organic light-emitting diodes, W. Stampor	256 (2000) 351
<i>Surfaces</i>	
Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco	256 (2000) 259
Microscopic and mesoscopic systems	
<i>Single atoms, molecules and assemblies (incl. biological)</i>	
Gas-phase measurement of ΔH^0 between axial and equatorial conformations of 3-methylcyclopentanone, D. Kim and T. Baer	256 (2000) 251
<i>Molecules (neutral and ionic)</i>	
Hartree-Fock crystal orbital calculation on sodium-intercalated fullerenes C ₆₀ Na ₁₀ and C ₆₀ Na ₁₁ , E.B. Starikov	256 (2000) 149
Prediction of pure electric-dipole two-photon absorption circular dichroism in lanthanide compounds, S. Naguleswaran, M.F. Reid and G.E. Stedman	256 (2000) 207

Determination of population, orientation and alignment of symmetric top molecule using laser-induced fluorescence, S.-L. Cong, K.-L. Han, G.-Z. He and N.-Q. Lou	256 (2000) 225
Photoelectron spectroscopy of vinylbromide and intramolecular dynamics of the ionic \tilde{B} state, A. Hoxha, R. Locht, B. Leyh, D. Deharenq, K. Hottmann and H. Baumgärtel	256 (2000) 239
<i>-diatomic</i>	
Theoretical study of the electronic structure of the LiRb and NaRb molecules, M. Korek, A.R. Allouche, M. Kobeissi, A. Chaalan, M. Dagher, K. Fakherdin and M. Aubert-Frécon	256 (2000) 1
<i>-small polyatomics</i>	
Systematic computational study of the geometrical dependence of deuterium quadrupole interaction parameters in an $O^-^2H \cdots O=C$ hydrogen bonded system, G.W. Turner, R.L. Johnston and K.D.M. Harris	256 (2000) 159
Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide, D.-Y. Hwang and A.M. Mebel	256 (2000) 169
<i>-aromatics</i>	
Photo-physical characterization of rhodamine 6G in a 2-hydroxyethyl-methacrylate methyl-methacrylate copolymer, W. Holzer, H. Gratz, T. Schmitt, A. Penzkofer, A. Costela, I. García-Moreno, R. Sastre and F.J. Duarte	256 (2000) 125
Ultrafast electron transfer in acceptor substituted bianthryl derivatives, M. Jurczok, P. Plaza, W. Rettig and M.M. Martin	256 (2000) 137
First hyperpolarizabilities of dipolar photoconductive chromophores: an approach toward monolithic molecular materials for photorefractivity, S. Kim, H. Moon, J. Hwang, J. Sohn, J. Seo, S.Y. Park, T. Im Kang and B. Rae Cho	256 (2000) 289
<i>-polymeric and biological</i>	
Structure-function self-organization in nonequilibrium macromolecular systems, L.N. Christophorov, A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik	256 (2000) 45
Density functional theory studies of methylated uracil: geometries and energies, C.F. Zhang, X.J. Chen, Z.S. Yuan, Z.J. Zhang and K.Z. Xu	256 (2000) 275
<i>-dimers</i>	
Systematic computational study of the geometrical dependence of deuterium quadrupole interaction parameters in an $O^-^2H \cdots O=C$ hydrogen bonded system, G.W. Turner, R.L. Johnston and K.D.M. Harris	256 (2000) 159
Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and supersonic jet-FTIR experiments, P. Asselin, P. Soulard, M.E. Alikhani and J.P. Perchard	256 (2000) 195
<i>-van der Waals molecules</i>	
New phenomena revealed by quantum chemical studies – the shellvation of GeH_3^+ by H_2 molecules, S. Roszak, P. Babinec and J. Leszczynski	256 (2000) 177
<i>-clusters</i>	
Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin	256 (2000) 61

New phenomena revealed by quantum chemical studies – the shellvation of GeH_3^+ by H_2 molecules, S. Roszak, P. Babinec and J. Leszczynski

256 (2000) 177

-complexes

Spectral properties and ligand field analysis of *cis*-dinitrito(1,4,8,11-tetraazacyclotetradecane)chromium(III) nitrate, J.-H. Choi

256 (2000) 29

Theoretical study of cation- π interactions of the metal complex cation, $[\text{Co}(\text{NH}_3)_6]^{3+}$, with ethylene and acetylene, S.D. Zarić

256 (2000) 213

Free radicals (incl. hydronium and muonium)

Theoretical study of the infrared and ultraviolet spectrum of the radical F_2CN , H. Dupin, I. Baraille, C. Larrieu and A. Dargelos

256 (2000) 7

Li cation-aromatic organic radical complex in a zeolite studied by electron spin echo envelope modulation spectroscopy, D.C. Doetschman, D.C. Gilbert and D.W. Dwyer

256 (2000) 37

Primary steps of an electron-proton reaction in aqueous electrolyte solutions, Y. Gauduel and H. Gelabert

256 (2000) 333

Ions and charge carriers

Li cation-aromatic organic radical complex in a zeolite studied by electron spin echo envelope modulation spectroscopy, D.C. Doetschman, D.C. Gilbert and D.W. Dwyer

256 (2000) 37

Proteins

DFT studies on helix formation in *N*-acetyl-(L-alanyl)_n-N'-methylamide for $n = 1-20$, M. Elstner, K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and S. Suhai

256 (2000) 15

Phenomena

Molecular structure

Theoretical study of the electronic structure of the LiRb and NaRb molecules, M. Korek, A.R. Allouche, M. Kobeissi, A. Chaalan, M. Dagher, K. Fakherdin and M. Aubert-Frécon

256 (2000) 1

Theoretical study of the infrared and ultraviolet spectrum of the radical F_2CN , H. Dupin, I. Baraille, C. Larrieu and A. Dargelos

256 (2000) 7

DFT studies on helix formation in *N*-acetyl-(L-alanyl)_n-N'-methylamide for $n = 1-20$, M. Elstner, K.J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and S. Suhai

256 (2000) 15

New phenomena revealed by quantum chemical studies – the shellvation of GeH_3^+ by H_2 molecules, S. Roszak, P. Babinec and J. Leszczynski

256 (2000) 177

Theoretical investigation on the potential energy surface for the reactions of B, Al and Ga with NO, L. Zhang and M. Zhou

256 (2000) 185

Investigation of the gas phase infrared spectrum of HF complexed with dimethyl ether from both cell- and supersonic jet-FTIR experiments, P. Asselin, P. Soulard, M.E. Alikhani and J.P. Perchard

256 (2000) 195

Gas-phase measurement of ΔH° between axial and equatorial conformations of 3-methylcyclopentanone, D. Kim and T. Baer

256 (2000) 251

Density functional theory studies of methylated uracil: geometries and energies, C.F. Zhang, X.J. Chen, Z.S. Yuan, Z.J. Zhang and K.Z. Xu	256 (2000) 275
<i>Vibrations and rotations of molecules</i>	
Theoretical study of the electronic structure of the LiRb and NaRb molecules, M. Korek, A.R. Allouche, M. Kobeissi, A. Chaalan, M. Dagher, K. Fakherddin and M. Aubert-Frécon	256 (2000) 1
Polarized Raman spectra of a single crystal of iodine, A. Congeduti, M. Nardone and P. Postorino	256 (2000) 117
Theoretical investigation on the potential energy surface for the reactions of B, Al and Ga with NO, L. Zhang and M. Zhou	256 (2000) 185
<i>Electronic structure and states</i>	
Theoretical study of the electronic structure of the LiRb and NaRb molecules, M. Korek, A.R. Allouche, M. Kobeissi, A. Chaalan, M. Dagher, K. Fakherddin and M. Aubert-Frécon	256 (2000) 1
Theoretical study of the infrared and ultraviolet spectrum of the radical F ₂ CN, H. Dupin, I. Baraille, C. Larrieu and A. Dargelos	256 (2000) 7
Hartree–Fock crystal orbital calculation on sodium-intercalated fullerites C ₆₀ Na ₁₀ and C ₆₀ Na ₁₁ , E.B. Starikov	256 (2000) 149
Theoretical investigation on the potential energy surface for the reactions of B, Al and Ga with NO, L. Zhang and M. Zhou	256 (2000) 185
Electronic energy dynamics of photoexcited ternary Zintl phase LiSbTe ₂ and the distance estimation between trap sites, S.-G. Kang, W.-S. Chae, Y.-R. Kim, J.-S. Jung and S.-H. Lee	256 (2000) 295
<i>Molecular interactions</i>	
Polarized Raman spectra of a single crystal of iodine, A. Congeduti, M. Nardone and P. Postorino	256 (2000) 117
Systematic computational study of the geometrical dependence of deuterium quadrupole interaction parameters in an O– ² H···O=C hydrogen bonded system, G.W. Turner, R.L. Johnston and K.D.M. Harris	256 (2000) 159
<i>Spectral bandshapes and intensities</i>	
Spectral density of medium strength H-bonds. Direct damping and intrinsic anharmonicity of the slow mode. Beyond adiabatic approximation, P. Blaise and O. Henri-Rousseau	256 (2000) 85
<i>Coupling of electronic and nuclear motion</i>	
Primary steps of an electron–proton reaction in aqueous electrolyte solutions, Y. Gauduel and H. Gelabert	256 (2000) 333
<i>Energy transfer processes</i>	
Time-resolved Fourier transform infrared spectroscopy of optically pumped carbon monoxide, E. Plönjes, P. Palm, A.P. Chernukho, I.V. Adamovich and J. William Rich	256 (2000) 315

Molecular photophysical processes

Electromodulation of fluorescence in hole-transporting materials (TPD, TAPC) for organic light-emitting diodes, W. Stämpfli

256 (2000) 351

Photochemistry

Light intensity dependence of a two-photon catalytic cycle: photoionization via absorption-electron transfer-absorption, M. Goez and V. Zubarev

256 (2000) 107

Intramolecular dynamics

Ultrafast electron transfer in acceptor substituted bianthryl derivatives, M. Jurczok, P. Plaza, W. Rettig and M.M. Martin

256 (2000) 137

Photoelectron spectroscopy of vinylbromide and intramolecular dynamics of the ionic \tilde{B} state, A. Hoxha, R. Locht, B. Leyh, D. Dehareng, K. Hottmann and H. Baumgärtel

256 (2000) 239

Luminescence spectra, yields and lifetimes

Spectral properties and ligand field analysis of *cis*-dinitrito(1,4,8,11-tetraazacyclotetradecane)chromium(III) nitrate, J.-H. Choi

256 (2000) 29

Photo-physical characterization of rhodamine 6G in a 2-hydroxyethyl-methacrylate methyl-methacrylate copolymer, W. Holzer, H. Gratz, T. Schmitt, A. Penzkofer, A. Costela, I. García-Moreno, R. Sastre and F.J. Duarte

256 (2000) 125

Electromodulation of fluorescence in hole-transporting materials (TPD, TAPC) for organic light-emitting diodes, W. Stämpfli

256 (2000) 351

Coherence loss processes

Direct simulation of non-linear interparticle collisional relaxation of ensembles of two-level systems, S. Longo, D. Bruno and P. Minelli

256 (2000) 265

Nonlinear responses (incl. optical)

Prediction of pure electric-dipole two-photon absorption circular dichroism in lanthanide compounds, S. Naguleswaran, M.F. Reid and G.E. Stedman

256 (2000) 207

First hyperpolarizabilities of dipolar photoconductive chromophores: an approach toward monolithic molecular materials for photorefractivity, S. Kim, H. Moon, J. Hwang, J. Sohn, J. Seo, S.Y. Park, T. Im Kang and B. Rae Cho

256 (2000) 289

Isolated molecules

Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide, D.-Y. Hwang and A.M. Mebel

256 (2000) 169

Electron transfer

Light intensity dependence of a two-photon catalytic cycle: photoionization via absorption-electron transfer-absorption, M. Goez and V. Zubarev

256 (2000) 107

Ultrafast electron transfer in acceptor substituted bianthryl derivatives, M. Jurczok, P. Plaza, W. Rettig and M.M. Martin

256 (2000) 137

Proton and hydrogen atom transfer

Primary steps of an electron-proton reaction in aqueous electrolyte solutions, Y. Gauduel and H. Gelabert

256 (2000) 333

Positron annihilation

Size of sodium dodecyl sulphate micelles in aqueous NaCl solutions as studied by positron annihilation lifetime spectroscopy, F. Bockstahl, E. Pachoud, G. Duplâtre and I. Billard

256 (2000) 307

-adsorption

Theoretical prediction of a carrier gas effect under nucleation in thermal diffusion chambers, A.L. Itkin

256 (2000) 61

-adsorbate structure

Li cation-aromatic organic radical complex in a zeolite studied by electron spin echo envelope modulation spectroscopy, D.C. Doetschman, D.C. Gilbert and D.W. Dwyer

256 (2000) 37

Thermodynamic and transport properties

Gas-phase measurement of ΔH^θ between axial and equatorial conformations of 3-methylcyclopentanone, D. Kim and T. Baer

256 (2000) 251

Critical behaviour and phase transitions

Order and disorder signatures in the specular scattering intensity of He particles from adsorbate covered Pt surfaces, G. Petrella, L. Cassidei and F. Ciriaco

256 (2000) 259

Molecular self-assembly and -organization

Structure-function self-organization in nonequilibrium macromolecular systems, L.N. Christophorov, A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik

256 (2000) 45

Biomolecular structure-function relationships

Structure-function self-organization in nonequilibrium macromolecular systems, L.N. Christophorov, A.R. Holzwarth, V.N. Kharkyanen and F. van Mourik

256 (2000) 45